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Ionized helium induced ionization of atomic hydrogen

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Abstract : Total and differential ionization cross sections of atomic hydrogen by impact of ionized helium in the energy range between 28 to 114 keV have been reported. We have applied a perturbative approach which accounts for the distortion due to the Coulomb fields of the projectile as well as of the residual target on equal footing. The present results, on comparing with the other existing theoretical predictions and measured data, are found to be encouraging

Keywords Atomic hydrogen, ionization by impact of structured projectile (He^+), calculations for collision energies 28 to 114 keV.

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Introduction

Ionization of atomic hydrogen by charged particles, primarily by proton and ionized helium has been a subject of continuing investigations for several decades. Much theoretical and experimental efforts have been put forth and marked progress have been made in understanding ion-atom/ion collisions. Ionization occurring as a result of structured projectile impact is considerably more complex than the impact of bare projectiles. This is due to the presence of bound electron(s) in the projectile. These electrons affect largely the process of ionization in many different ways, such as, they may screen the incoming nuclear charge and may be excited to discrete or continuum state. From theoretical point of view this complicates the problem and therefore calculations must be performed that include each of the reaction pathways [1], namely target ionization resulting from collisions where the projectile is simultaneously excited, target ionization with the restriction that the projectile remains in the ground states, projectile ionization with the target remains in ground state and projectile ionization with simultaneous ionization of target. Practically it is a difficult task to perform calculations which accounts for all these reaction channels.

The theoretical description of collision problems involving ion-atom/ion collisions is of great interest because it provides a benchmark for understanding the processes in detail. Moreover, it involves many interaction phenomena which need to be studied in deep details. In this direction the works of Y Y Hsu *et al* [2] is much enthusiastic. It is both theoretical as well as experimental work on $He^+ + H$ system in the energy range 28–114 keV, the results have been compared with the existing theoretical results [2]. However, a close look at the comparison data shows a wide difference between the experimental and the theoretical works, expecially at the low energy region. Such difference evolved much interest in the present work where we have studied the same system, *i.e*, He^+-H, in a somewhat different manner.

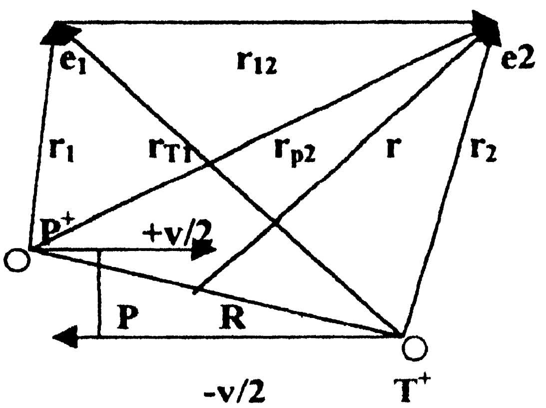
A general three body problem in ion-atom collision has been extensively treated by various authors of Refs. [3–6]. But the proposed system is a four body one and involves many complexities due to the presence of bound electron(s). However in Refs. [7–9] have taken up the matter quite efficiently and have found results for fast projectiles. A perturbative approach to the problem has already been suggested by Inokuti [10] which involves high impact

*Institute of Material Science, University of Tsukuba, Ibaraki-305 8573, Japan velocities or small projectile charges. But for fast collisions when the projectile charges are of the order of the target nuclear charge or even greater a more comprehensive theory is required Reinhold *et al* [11] modified the clssical trajectory Monte Carlo (CTMC) method to cope with the above requirements and applied it for p-H/He system. Their results are quite in agreement with experimental data.

In this work we have attempted to study the ionization process of He^{+} + H system, where we calculate the total and differential ionization cross sections. In Section 2, we describe the theory in brief and in Section 3 we present the results and discussions.

2. Theory

The collision system in the present study is a complex one since the projectile contains an electron which needs to be treated properly.



(Coordinates for He^{+}–H collision system)

We solve the one-electron Schrödinger equation for the system with electronic Hamiltonian

$$H_e = -\frac{1}{2}\nabla_r^2 + V_T(r_2) + V_P(r_1) + \frac{1}{r_{12}} \tag{1}$$

(atomic units are used throughout),

where $r_1(r_2)$ is the distance of the electrons corresponding to the nuclei of projectile (target) and r_{12} is the distance between the two electrons. We adopt here the impact parameter formalism, where the inter-nuclear motion is treated classically as $\boldsymbol{R} = \boldsymbol{p} + \boldsymbol{v}t$ in which $\boldsymbol{p}$ is the impact parameter, $\boldsymbol{v}$ is the relative velocity of the projectile with the target, and the midpoint of the line joining the two nuclei is chosen as the origin. Time is measured from the instant when the two nuclei are the closest to each other.

The development in time t of the transition amplitude for ionization with the ejection of an electron from the target with momentum $\boldsymbol{k}$ can be written as

$$\frac{d}{dt}(c_k(p)) = \int\left[\Psi_f^{-*}\left(H_e - i\frac{d}{dt}\right)\Psi_i\right]dr, \tag{2}$$

with the initial condition that at $t = -\infty$, $c_k = 0$. The ionization probability is $|c_k(t = +\infty)|^2$.

We consider the continuum state wave function in which the Coulomb fields due to the projectile and the residual target are taken on equal footing. It may be pointed out that this condition is a good approximation for intermediate energy collision.

For the final continuum state wave function we write :

$$\psi_{\bar{k}_e}^{-} = N_1 N_2 e^{ik\cdot r}\, {}_1F_1\left(i\alpha_p, 1; -i(k_p r_p + \boldsymbol{k}_p\cdot \boldsymbol{r}_p)\right)$$

$$\times\, {}_1F_1\left(i\alpha_T, 1; -i(k_T r_T + \boldsymbol{k}_T\cdot\boldsymbol{r}_T)\right) e^{-i\frac{k^2 t}{2}}, \tag{3}$$

where $\alpha_p = -\frac{Z_p}{k_p}$ and $\alpha_T = -\frac{Z_T}{k_T}$;

and $N_1 = e^{-\pi\alpha_p/2}\Gamma(1 + i\alpha_p)$, $N_2 = e^{-\pi\alpha_T/2}\Gamma(1 + i\alpha_T)$

Finally we can write the electron bound continuum state wave function as

$$\Psi_f^{-} = \phi_i(r_1) \times \psi_{\bar{k}_e}^{-}. \tag{3a}$$

The initial state wave function used in the present approach is as follows :

$$\Psi_i = \phi_i(r_1) \times \phi_i'(r_2) \tag{3b}$$

where $\phi_i(r_1)$ is the electronic wave function of the projectile (He^{+}) in its ground state and $\phi_i'(r_2)$ is the electronic wave function of the target (H) in its ground state.

Where $\phi_i(r_1) = \frac{2^{3/2}}{\sqrt{\pi}} e^{(-z r_1)} e^{\left(-i\varepsilon_{He^+} t - \frac{i}{8}v^2 t\right)} e^{i\frac{v}{2}\cdot r_1}$

$$\phi_i'(r_2) = \frac{1}{\sqrt{\pi}} e^{(-z r_2)} e^{\left(-i\varepsilon_H t - \frac{i}{8}v^2 t\right)} e^{-i\frac{v}{2}\cdot r_2}$$

The above final-state wave function asymptotically satisfies the Schrödinger equation,

$$-\frac{1}{2}\nabla_r^2 - \frac{Z_P}{r_1} - \frac{Z_T}{r_2} + \frac{1}{r_{12}} - i\frac{\partial}{\partial t}\,|\Psi_f^{-} = 0. \tag{4}$$

The doubly differential cross sections may be written as

$$\frac{d^2\sigma}{dE_e d\Omega_e} = k\int d^2 p |C_k(p)|^2$$

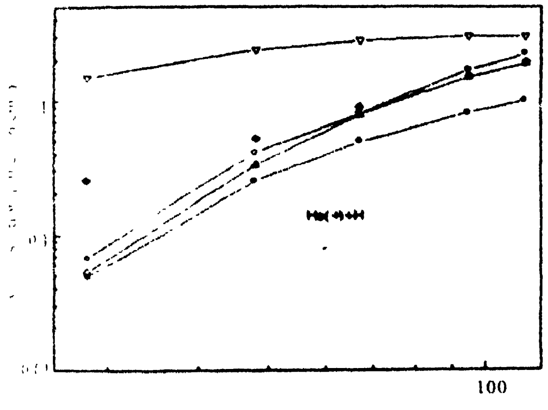
and the total ionization cross sections (σ_{total}) are calculated by using the following integral,

$$\sigma_{total} = 2\pi\int \frac{d^2\sigma}{dE_e d\Omega_e}\sin\theta_e d\theta_e dE_e$$

(Symbols have their usual meanings).

Results and discussions

ure 1. displays the total ionization cross sections for ation of hydrogen atom by impact of ionized helium. have also displayed in the same figure the cross section ues of other theoretical calculations as well as the sured data of Ref. [2] for comparison. It may be seen m the figure that the present results are found to be in sonably good agreement with the experimental data of f [2] as well as with the calculated values of continuum orted wave-eikonal initial state (CDW-EIS) approximation above 65 keV impact energy. Below this energy the sent result although found to be slightly higher in nitude than the CDW-EIS values, maintains the trend. wever, there is a marked disagreement between the erimental data and the results calculated by the present ory as well as other existing theoretical values.



re 1. Total ionization cross section of atomic hydrogen by impact nized helium. Present results : (—o—), CTMC results (Ref. [2]) :), CDW-EIS results (Ref. [2]) : (—Δ—), Born results (Ref. [2])) experimental data (Ref. [2] : (♦♦♦♦♦).

The results calculated by using Born approximation are nd to be of much higher in magnitude than the calculated lts as well as the experimental data. The present results ound to be of higher in magnitude in comparison with MC values throughout the energy range considered.

t may be seen from the figure that none of the theoretical es presented in the figure interpret well the experimental in the low energy region. This clearly signifies the sion of contributions from different reaction channels h are important especially in the low energy collision.

An interesting feature to be noted in Figure 2 is the re of variation of the ratio of total ionization cross on of hydrogen atom by impact of He^{++} to that for He^{+} in the incident energy range 28 to 114 keV. It is evident the figure that there is a tendency of the curve to reach y as the energy increases. However, at low energy region the ratio is quite high. Thus it is immediately apparent that at low energy the probability for collision with atomic

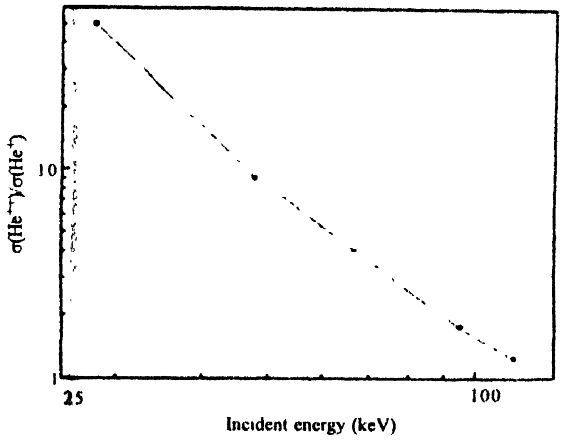


Figure 2. Ratio of total ionization cross sections of atomic hydrogen by alpha particle and ionized helium impact as a function of collision energy. Present result . (—•—).

hydrogen by the impact of bare projectile is far more greater than that for structured projectile; while at high energy the probability for the two are almost same. This is indicative that though at high energy region the structured and bare projectiles may be treated on equal footing, but the situation is different at low energy region. Since during slow collision many inelastic channels strongly couple with one another open up, exchanging flux and phase in a quite complex manner. Thus without simultaneous inclusion of important channels, an accurate determination of cross sections is not possible during slow collisions.

Figure 3 presents the doubly differential cross sections (DDCS) as a function of electron ejection energy by 114 keV He^{+} impact on atomic hydrogen for a fixed ejection angle of

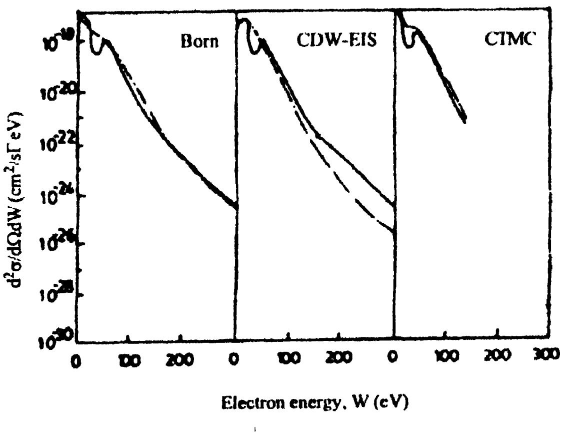


Figure 3. Doubly differential ionization cross sections of atomic hydrogen by impact of 114 keV ionized helium as a function of electron energy at ejection angle 15°. Present results : (—), Born (Ref. [2]) : (—•—), CDW-EIS (Ref. [2]) : (—•—), and CTMC (Ref. [2]) : (—•—).

15°. The present results on comparison with the values calculated by the first Born approximation are found to be slightly smaller in magnitude at intermediate electron energies but coincide at higher energies. In comparison with the results of CDW-EIS, the present values are found to achieve reasonable good agreement up to a certain energy range but overestimate at higher energies. The present results also show both quantitative and qualitative agreement with the CTMC results. It may be seen from the figure that the present results show a structure in cross section around 25 eV ejection energy which is also present in the CTMC results. However, both the CDW-EIS and the Born values do not show any structure in the spectra.

4. Conclusion

The present calculated results for differential ionization cross sections are found to be of reasonably accord with other theoretical values. However, in case of total ionization cross sections, it may be found from Figure 1 that none of the theoretical methods are able to interpret the experimental data especially in the low incident energy. This phenomena clearly invites the sophisticated theoretical models which should include the calculations for each of the several reaction pathways mentioned earlier in addition to the captu channel. This channel becomes particularly important in low to intermediate energy region. In the present case th collision of He^{+}–H is an accidental resonating system wh both the reactants are in ground state.

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